Electron Affinity of Some Conventional and Trimetallic Nitride Endohedral Metallofullerenes

Lev N. Sidorov,¹ Olga V. Boltalina,¹ Ilya N. Ioffe,¹ Arseny S. Ievlev,¹ Harry C. Dorn,² Steve Stevenson³ and Robert D. Bolscar⁴

¹Moscow State University Chemistry Department Vorobyovy Gory Moscow 119899 Russia

²Virginia Polytechnic Institute and State University Department of Chemistry Blacksburg, VA 24061 USA

> ³Luna NanoMaterials P.O. Box 11704 Blacksburg, VA 24061 USA

⁴TDA Research, Inc. 12345 West 52nd Avenue Wheat Ridge, CO 80033 USA

The electron exchange reactions involving fullerenes and endohedral metallofullerenes containing various lanthanide and III group metal atoms, including the species from the trimetallic nitride family $(M_3N@C_{80})$, were studied by means of the Knudsen Cell Mass Spectrometry Ion-Molecular Equilibria method, and the equilibrium constants of these reactions were determined. We report the electron affinity values of some mono-, di-, and trimetallic nitride metallofullerenes derived from the Gibbs energies of electron exchange reactions, electron affinities of some higher fullerenes being taken as reference. It was found that mono- and even dimetallofullerenes are stronger electron acceptors than the corresponding hollow fullerenes despite the charge transfer to the carbon cage. In some cases, electron affinity increase may be accounted for by the differences in the hollow and endohedral fullerenes isomerism, the latter being caused by the permutations in the relative stability order of the carbon cage after endohedral atoms entrapping. On the contrary, the molecules from the trimetallic nitride family reveal lower electron affinity than those of the hollow higher fullerenes, possibly due to the higher value of the total charge transfer from the metal atoms to the carbon cage in compare with the mono- and dimetallo-

fullerene molecules.